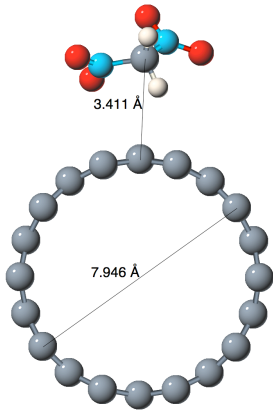
Molecular dynamics of laser assisted decomposition of unstable molecules at the surface of carbon nanotubes

Brendon Disrud, Yulun Han, Dmitri Kilin

Department of Chemistry and Biochemistry, North Dakota State University Fargo, ND

Carbon nanotubes (CNTs) have affinity to adsorb several classes of molecules, ranging from small inorganic molecules to biological polymers, DNA, and conjugated polymers.[1] Such functionalization allows tuning of optoelectronic properties of CNTs, e.g. enhance their photoluminescence. The cleaning of CNTs from functional agents is often a challenge. We explore the hypothesis that desorption of molecules from CNT surface can be controlled by UV-vis photoexcitations. In addition, we test a hypothesis that presence of CNT substrate can facilitate several chemical reactions such as photodegradation of molecules, related to optically controlled explosion.[2] The laser assisted desorption and decomposition is explored by recently developed time dependent excited state molecular dynamics (TDESMD) methodology, which takes into account simultaneous evolution of electronic excitation, nuclear positions, under periodic optical excitation.[3] The approaches are tested on dinitromethane molecule adsorbed to (10,0) CNT.[4] This model demonstrates potential of photoinduced charge transfer between adsorbate and substrate, which can affect efficiency of desorption and decomposition reactions.



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